Example 1b

June 17, 2020

1 Example 1b: Harmonic trap - Analyzing experimental data with pretrained network

Example code to analyze experimental data with DeepCalib using a pretrained network.

DeepCalib 1.0 Enhanced force-field calibration via machine learning version 1.0 - 27 April 2020 l' Aykut Argun, Tobias Thalheim, Stefano Bo, Frank Cichos & Giovanni Volpe Soft Matter Lab

1.1 1. INIZIALIZATION

```
In [1]: import DeepCalib
```

1.2 2. Import and visualize the experimental trajectory to be analyzed

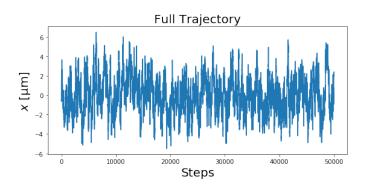
Here we import and visualize the experimental trajectory.

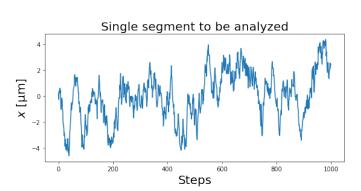
Comments: 1. Make sure you define the same scaling functions for the inputs and the targets the same in the training file.

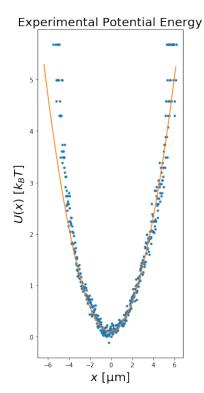
```
In [2]: \#\#\# Import the data
        ### Example 1a
        import scipy.io as sci
        data_name = 'Data_Example1b'
        x = sci.loadmat(data_name)['x'].reshape(50000,)
        ### Visualize the trajectory
        import matplotlib.pyplot as plt
        %matplotlib inline
        fig = plt.figure(figsize=(15, 10))
        gs = fig.add_gridspec(10,10)
        plt.subplot(gs[0:4,0:6])
        plt.ylabel('$x$ [\u03BCm]',fontsize=20)
        plt.xlabel('Steps',fontsize=20)
        plt.title('Full Trajectory',fontsize=20)
        plt.plot(x)
        ### Visualize a single input for analysis
```

```
plt.subplot(gs[6:10,0:6])
plt.ylabel('$x$ [\u03BCm]',fontsize=20)
plt.xlabel('Steps',fontsize=20)
plt.title('Single segment to be analyzed',fontsize=20)
plt.plot(x[23000:28000:5])
### Visualize the measured truths
import numpy as np
1 = (np.arange(500) - 250) * 0.025
h = np.histogram(x, bins = 1)[0]
U = -np.log(h[h>0]) + np.log(h[round(h.size/2)])
plt.subplot(gs[:,7:10])
plt.xlabel('$x$ [\u03BCm]',fontsize=20)
plt.ylabel('$U(x)$ [$k_BT$]',fontsize=20)
plt.title('Experimental Potential Energy',fontsize=20)
plt.plot(l[np.append(h>0,False)],U,'.')
k = 1.1
                                                                   # Measured stiffness
from scipy.constants import Boltzmann as kB
plt.plot(1-.1, .5*k*1e-9*l**2*1e-12/kB/300 + .1)
```

Out[2]: [<matplotlib.lines.Line2D at 0x240ab3af860>]







```
In [4]: ### Analyze the data
        from keras.models import load_model
        import numpy as np
        from scipy.constants import Boltzmann as kB
        network = load_model('Network_Example_1a.h5')
        predictions_k = []
        oversamp = 1
        nmeas = 400
        steps = int((x.size-1000*oversamp)/nmeas)
        slength = 1000*oversamp
        for i in range(nmeas):
            x_crop = x[(i*steps):(i*steps+slength):oversamp]
            predicted_k = DeepCalib.predict(network, x_crop)[0]
            predictions_k.append(predicted_k)
        k0 = 10
        rescale_targets = lambda scaled_k: np.exp(scaled_k) * k0  # Inverse of targets_scaling
In [5]: ### Plot the results
        fig = plt.figure(figsize=(10, 5))
        plt.plot(rescale_targets(predictions_k),'.')
        plt.plot([0, nmeas], np.array([k, k]),color='black')
        plt.ylim([0, 5])
        plt.xlabel('Trajectory Segments',fontsize=20)
        plt.ylabel('Measured $k$ [fN/\u03BCm]',fontsize=20)
Out[5]: Text(0, 0.5, 'Measured $k$ [fN/m]')
     Measured k [fN/\mum]
        0
                     50
                            100
                                            200
                                                     250
                                                             300
                                                                     350
                                                                             400
```

Trajectory Segments